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Stochastic delineation of well capture zones

Abstract In this work, we describe a stochastic method for delineating well capture zones in randomly heterogeneous porous media. We use a moment equation (ME) approach to derive the time-dependent mean capture zones and their associated uncertainties. The mean capture zones are determined by reversely tracking the non-reactive particles released at a small circle around each pumping well. The uncertainty associated with the mean capture zones is calculated based on the particle displacement covariances for nonstationary flow fields. The flow statistics are obtained either by directly solving the flow moment equations derived with a first-order ME approach or from Monte Carlo simulations (MCS) of flow. The former constitutes a full ME approach, and the latter is a hybrid ME-MCS approach. This hybrid approach is invoked to examine the validity of the transport component of the stochastic method by ensuring that the ME and MC transport approaches have the same underlying flow statistics. We compared both the full ME and the hybrid ME-MCS results with those obtained with a full MCS approach. It has been found that the three approaches are in excellent agreement when the variability of hydrologic conductivity is small ($\sigma_Y^2 = 0.16$). At a moderate variability ($\sigma_Y^2 = 0.5$), the hybrid ME-MCS and the full MCS results are in excellent agreement whereas the results from the full ME approach deviate slightly from the full MCS results. This indicates that the (first-order) ME transport approach renders a good approximation at this level of variability and that the first-order ME flow approximation may not be sufficiently accurate at this variability in the case of divergent/convergent flow. The first-order ME flow approach may need to be corrected with higher-order terms even for moderate σ_Y^2 although the literature results reveal that the first-order ME flow approach is robust for uniform mean flow (i.e., giving accurate results even with σ_Y^2 as large as four).

Keywords Stochastic method · Capture zone Heterogeneity · Nonstationary · Moment equation approach · Monte Carlo simulation

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1 Introduction

An accurate description of well capture zones plays an important role in well-head protection and designing remediation systems for contaminated aquifers. Many models have been developed in delineating well capture zones for flow in both homogeneous and heterogeneous porous media. Early models are based on the assumption that the permeability of the porous medium is homogeneous, which lead to analytical solutions. Bear and Jacobs (1965) derived an analytical equation for the isochrones of a fully penetrating well pumping in a confined aquifer with a uniform background hydraulic gradient. Javandel and Tsang (1987) provided capture-zone type curves for several well placement configurations. Other analytical models for capture zones are available for confined and unconfined aquifers (Grubb, 1993), recharged aquifer systems Lerner (1992), a double well system (pumping-pumping and pumping-injection) (Zhan, 1998), two arbitrarily located wells (Shan, 1999), and horizontal wells (Zhan, 1999). Bhatt (1993) investigated the influence of the main aquifer properties, such as effective porosity and saturated thickness, on the transverse and longitudinal extent of a capture zone in a confined aquifer. Some other factors that influence the capture zone geometry have been studied including aquifer anisotropy (Schafer, 1996; Bair and Lahm, 1996; Zlotnik, 1997) and partial penetration of pumping wells (Bair and Lahm, 1996; Zlotnik, 1997).

In the recent years, with the Monte Carlo method several studies have considered the variability of medium properties in delineating the well capture zone

(Varljen and Shafer, 1991; Bair et al., 1991; Cole and Silliman, 1997; Franzetti and Guadagnini, 1996; Guadagnini and Franzetti, 1999; Riva et al., 1999; van Leeuwen et al., 1998). There are several problems with this probability-based approach in delineating well capture zones. The computation effort in this approach can be very large. For each Monte Carlo realization, a particle is released at all grid nodes, requiring numerical computation of a particle trajectory starting from each node until the particle either is captured by the well or reaches the boundary of the flow domain. This algorithm could be even more cumbersome for a system with multiple wells. The limitation of Monte Carlo simulations has been discussed in the literature (e.g., Neuman, 1997; Guadagnini and Neuman, 1999; Zhang, 2002): the lack of convergence criteria and the requirement of high computational efforts, among others. The computational demand is even large if there are uncertainties in boundary and initial conditions.

Kunstmann and Kinzelbach (2000) computed the capture zones using the first-order second moment method on the basis of a Eulerian framework. They derived moment equations for flow and transport equations, and the mean capture zone was defined as the concentration isoline of $c = 0.5$ and the confidence intervals are determined by plus or minus a few standard deviations of concentration. One problem with this algorithm is that it works only for a single well, because in the case of multiple wells it is difficult to distinguish the contributions of different wells to the concentration field. In such a situation, the concentration isoline of $c = 0.5$ may not be appropriate to define the mean capture zones. It is seen from their examples for the cases with a single well that the mean capture zones and the associated confidence intervals are not in good agreement with Monte Carlo simulation results for the unconditional case, even though the variance of the log transmissivity is as low as 0.16.

Recently, Stauffer et al. (2002) briefly reported an investigation on the uncertainty quantification of the well capture zones and well catchments in heterogeneous media using a first-order approximation. Specifically, the capture zone of a well for a given time is determined by backward movement of many particles starting near the well, and the uncertainty bandwidth of capture zones is approximated using longitudinal and transversal particle displacement covariances along and normal to the mean particle trajectory. One of limitations in their work is that the nonstationary velocity covariances were approximated by locally scaling the stationary velocity covariance derived by Rubin (1990) for uniform mean flows.

Based on a general stochastic model developed for advective transport of conservative solutes in variably saturated multi-dimensional nonstationary flow in randomly heterogeneous porous media (Lu and Zhang, 2003a), Lu and Zhang (2003b) present a moment equation (ME) based stochastic approach to delineate the well capture zones for a system with an arbitrary number of wells (either pumping or injection). A certain number of particles are released around each pumping well in the (first-order) mean flow field and the reverse particle tracking is performed. The first-order mean capture zones are delineated using the first-order mean flow velocity. The confidence intervals of capture zones are derived from the particle displacement covariances for nonstationary flows (Lu and Zhang, 2003b), which are expressed in terms of the state transition matrix that satisfies a time-varying dynamic equation whose coefficient matrix is the derivative of the mean Lagrangian velocity field. For a strongly nonuniform flow field such as in the presence of pumping or injection wells, the computation of the state transition matrix is problematic. Lu and Zhang (2003b) proposed two simple approaches to compute the (first-order) state transition matrix for the case of statistically homogeneous porous media, i.e., using the exact solution for a rectangular domain or using the potential theory otherwise. For several cases with one or two pumping wells, they validated their transport model by comparing the scatter plots of particles' positions at given elapsed times from Monte Carlo simulations (MCS) against the mean capture zones with confidence intervals at the given times, and an excellent agreement is found between the model results and those from Monte Carlo simulations. However, their transport approach may be best called a hybrid ME-MCS approach in that the flow statistics to their transport model, i.e., the mean flow field and the velocity covariances, are computed from Monte Carlo simulations rather than from solving the flow moment equations.

The objective of this study is to investigate the efficiency and accuracy of the two methods in calculating the state transition matrix, and more importantly, to investigate the accuracy of a full ME approach. In this approach, the stochastic transport model is evaluated with the mean velocity and velocity covariances obtained from directly solving the flow moment equations rather than from Monte Carlo simulations as in the hybrid ME-MCS approach of Lu and Zhang (2003b).

2 Mathematical formulation

We consider transient flow in saturated porous media satisfying the following continuity equation and Darcy's law:

$$-\nabla \cdot \mathbf{q}(\mathbf{x}, t) + \sum_{j=1}^{n_w} Q_{jw}\delta(\mathbf{x} - \mathbf{x}_j) = S_s \frac{\partial h(\mathbf{x}, t)}{\partial t} \tag{1}$$

$$\mathbf{q}(\mathbf{x}, t) = -K(\mathbf{x})\nabla h(\mathbf{x}, t) \tag{2}$$

subject to initial and boundary conditions

$$\begin{aligned} &h(\mathbf{x}, 0) = h_0(\mathbf{x}) \quad \mathbf{x} \in \Omega \\ &h(\mathbf{x}, t) = h_1(\mathbf{x}, t) \quad \mathbf{x} \in \Gamma_D \\ &\mathbf{q}(\mathbf{x}, t) \cdot \mathbf{n}(\mathbf{x}) = Q(\mathbf{x}, t) \quad \mathbf{x} \in \Gamma_N \end{aligned} \tag{3}$$

where $\mathbf{q}$ is the specific discharge, $h(\mathbf{x}, t)$ is the hydraulic head, $h_0(\mathbf{x})$ is the initial head in the domain Ω, $h_1(\mathbf{x}, t)$ is the prescribed head on Dirichlet boundary segments Γ_D, $Q(\mathbf{x},t)$ is the prescribed flux across Neuman boundary segments Γ_N, $\boldsymbol{n}(\mathbf{x})$ is an outward unit vector normal to the boundary, S_s is the specific storage, $K(\mathbf{x})$ is the saturated hydraulic conductivity (assumed to be isotropic locally), n_w is the number of pumping (or injection) wells, and Q_{jw} is the pumping (or injection) rate of the jth well located at $\mathbf{x}_j$.

2.1 First-order moment equations

First-order moment equations for flow in unsaturated/saturated porous media have been developed by Zhang and Lu (2002) and Lu and Zhang (2002), and they can be easily reduced to equations for saturated flow. However, for completeness, here we briefly outline the procedure. For simplicity, we assume that porosity ϕ, specific storage S_s, and all boundary and initial conditions are deterministic. For random boundary and initial conditions, the readers are referred to Zhang and Lu (2002) or Lu and Zhang (2002) for details. Again, we assume that the hydraulic conductivity $K(\mathbf{x})$ follows a log normal distribution, and work with the log-transformed variable $Y(\mathbf{x}) = \ln(K(\mathbf{x})) = \langle Y(\mathbf{x})\rangle + Y'(\mathbf{x})$. One may express $h(\mathbf{x}, t)$ as an infinite series as $h(\mathbf{x}, t) = h^{(0)} + h^{(1)} + h^{(2)} + \cdot$ In this series, the order of each term is with respect to σ_Y, the standard deviation of $Y(\mathbf{x})$. After combining (1) and (2), substituting the expansions of $h(\mathbf{x}, t)$ and $Y(\mathbf{x})$, and collecting terms at separate order, one obtains the following equations governing the first two moments of head,

$$\frac{\partial^2 h^{(0)}(\mathbf{x},t)}{\partial x_i^2} + \frac{\partial\langle Y(\mathbf{x})\rangle}{\partial x_i}\frac{\partial h^{(0)}(\mathbf{x},t)}{\partial x_i} + \sum_{j=1}^{n_w}\frac{Q_{jw}}{K_G(\mathbf{x})}\delta(\mathbf{x}-\mathbf{x}_j) = \frac{S_s}{K_G(\mathbf{x})}\frac{\partial h^{(0)}(\mathbf{x},t)}{\partial t}$$

$$h^{(0)}(\mathbf{x},0) = \langle h_0(\mathbf{x})\rangle \quad \mathbf{x}\in\Omega$$

$$h^{(0)}(\mathbf{x},t) = \langle h_1(\mathbf{x},t)\rangle \quad \mathbf{x}\in\Gamma_D,\ \ t>0$$

$$n_i(\mathbf{x})\frac{\partial h^{(0)}(\mathbf{x},t)}{\partial x_i} = -\langle Q(\mathbf{x},t)\rangle/K_G(\mathbf{x}) \quad \mathbf{x}\in\Gamma_N,\ \ t>0 \quad (4)$$

$$\frac{\partial^2 C_h(\mathbf{x},t;\chi,\tau)}{\partial x_i^2} + \frac{\partial\langle Y(\mathbf{x})\rangle}{\partial x_i}\frac{\partial C_h(\mathbf{x},t;\chi,\tau)}{\partial x_i} = \frac{S_s}{K_G}(\mathbf{x})\frac{\partial C_h(\mathbf{x},t;\chi,\tau)}{\partial t} - \frac{\partial h^{(0)}(\mathbf{x},t)}{\partial x_i}\frac{\partial C_{Yh}(\mathbf{x};\chi,\tau)}{\partial x_i} - C_{Yh}(\mathbf{x};\chi,\tau)\left[\frac{\partial^2 h^{(0)}(\mathbf{x},t)}{\partial x_i^2} + \frac{\partial\langle Y(\mathbf{x})\rangle}{\partial x_i}\frac{\partial h^{(0)}(\mathbf{x},t)}{\partial x_i}\right]$$

$$C_h(\mathbf{x},0;\chi,\tau) = 0 \quad \mathbf{x}\in\Omega$$

$$C_h(\mathbf{x},t;\chi,\tau) = 0 \quad \mathbf{x}\in\Gamma_D, \quad t>0$$

$$n_i(\mathbf{x})\left[\frac{\partial C_h(\mathbf{x},t;\chi,\tau)}{\partial x_i} + C_{Yh}(\mathbf{x};\chi,\tau)\frac{\partial h^{(0)}(\mathbf{x},t)}{\partial x_i}\right] = 0 \quad \mathbf{x}\in\Gamma_N,\ \ t>0 \quad (5)$$

where K_G is the geometric mean, and $C_{Yh}(\chi;\ \mathbf{x},\ t)$ satisfies an equation similar to (5), replacing $C_{Yh}(\mathbf{x};\ \chi,\ \tau)$ and $C_h(\mathbf{x},t;\ \chi,\ \tau)$ in (5) by $C_Y(\mathbf{x};\ \chi)$ and $C_{Yh}(\chi;\ \mathbf{x},\ t)$, respectively. The first two moments of the flux are (Zhang, 2002)

$$\mathbf{q}^{(0)}(\mathbf{x},t) = -K_G(\mathbf{x})\nabla h^{(0)}(\mathbf{x},t)$$

$$\mathbf{C_q}(\mathbf{x},t;\chi,\tau) = K_G(\mathbf{x})K_G(\chi)\Big[C_Y(\mathbf{x},\chi)\nabla_{\mathbf{x}}h^{(0)}(\mathbf{x},t)\nabla_\chi^T h^{(0)}(\chi,\tau) + \nabla_{\mathbf{x}}h^{(0)}(\mathbf{x},t)\nabla_\chi^T C_{Yh}(\mathbf{x};\chi,\tau) + \nabla_{\mathbf{x}}C_{Yh}(\chi;\mathbf{x},t)\nabla_\chi^T h^{(0)}(\chi,\tau) + \nabla_{\mathbf{x}}\nabla_\chi^T C_h(\chi,\tau;\mathbf{x},t)\Big] \quad (6)$$

The first two moments of the velocity field can be derived from (6).

2.2 Mean trajectory and displacement covariances

For a given flow field, the trajectory of a particle located at $\mathbf{a}$ at $t = t_0$ is described by the kinematic equation, $d\mathbf{X}(t;\ \mathbf{a},\ t_0)/dt = \mathbf{V}[\mathbf{X}(t;\ \mathbf{a},\ t_0)]$, subject to the initial condition $\mathbf{X}(t_0;\ \mathbf{a},\ t_0) = \mathbf{a}$. Here $\mathbf{X}(t;\ \mathbf{a},\ t_0)$ stands for the particle position at time t and $\mathbf{V}[\mathbf{X}(t;\ \mathbf{a},\ t_0)]$ the (Lagrangian) velocity of the particle at t. The first-order mean trajectory $\langle\mathbf{X}_t\rangle$ and the displacement covariances have been given by Lu and Zhang (2003a) as

$$\frac{d\langle\mathbf{X}_t\rangle}{dt} = \langle\mathbf{V}[\langle\mathbf{X}_t\rangle]\rangle \quad (7)$$

$$\mathbf{X}_{ij} = \langle X'_{t,i}X'_{t,j}\rangle = \int_{t_0}^{t}\int_{t_0}^{t}\Phi_{ik}(t,\tau)\Phi_{jl}(t,\tau')\langle V'_k(\langle\mathbf{X}_\tau\rangle)V'_l(\langle\mathbf{X}'_\tau\rangle)\rangle d\tau d\tau' \quad (8)$$

Here $\Phi(t,\tau)$ is called the transition matrix (or fundamental matrix) satisfying $d\Phi(t,\ \tau)/dt = \boldsymbol{B}(t)\Phi(t,\ \tau)$ with initial condition $\Phi(\tau,\ \tau) = \mathbf{E}$, the identical matrix, and $\boldsymbol{B}(t)$ is the derivative of mean (Lagrangian) velocity $\langle\mathbf{V}[\langle\mathbf{X}_t\rangle]\rangle$ with respect to the mean trajectory $\langle\mathbf{X}_t\rangle$. In the case that the flow field is stationary and unidirectional, the state transition matrix $\Phi(t,\ \tau)$ equals the identical matrix and our expression recovers the well-known expression of Dagan (1984). For the nonuniform but unidirectional flow, $\Phi(t,\ \tau)$ becomes an exponential matrix function and our expression reduces to those of Butera and Tanda (1999) and Sun and Zhang (2000).

3 Numerical implementation

The moment equations in general cannot be solved analytically. Numerical implementation of these equations has been discussed in detail by Zhang and Winter (1998). Upon solving these moment equations, the first-order mean Eulerian velocity field and velocity covariances can be calculated. For a particle released at location $\mathbf{X}_0$ at time $t = 0$, the first-order mean Lagrangian velocity field and its covariances can be derived based on the first-order mean Eulerian velocity field and velocity covariances. The velocity field is then negated for reversed particle tracking. The mean trajectory up to first-order can be obtained by solving (7), using the negated velocity field. The derivatives of the first-order mean Lagrangian velocity field with respect to the mean trajectory (along the particle path), B_{ij}(t), can be calculated by numerically taking derivatives of the mean Lagrangian velocity field.

It is worthy to note that, in general, there is no simple analytical expression for the transition matrix $\Phi(t, \tau)$ (unless $\mathbf{B}$ is time-invariant or diagonal, which yields the respective result of $\Phi(t, \tau) = \exp[\mathbf{B}(t\text{-}\tau)]$ or $\Phi(t, \tau) = \exp\left[\int_\tau^t B(\tau')\mathrm{d}\tau'\right]$), the moments X_{ij} have to be evaluated numerically, which requires evaluation of the state transition matrix $\Phi(t, \tau)$ for certain values of t and τ . Lu and Zhang (2003a) proposed an algorithm to compute $\Phi(t, \tau)$. When the flow field is highly non-uniform, for example, in the presence of pumping or injection wells, it is difficult to calculate $\Phi(t,\tau)$ with desired accuracy, mainly due to errors introduced in numerically computing matrix $\mathbf{B}$.

In some special cases, however, the first-order approximation of the $\mathbf{B}$ matrix can be derived analytically, instead of calculating it numerically by taking derivatives of the first-order mean velocity field. Lu and Zhang (2003b) suggested two simple approaches to compute matrix $\mathbf{B}$. If the porous medium is statistically homogeneous and the flow domain is rectangular, the exact solution of the first-order steady-state mean head field (and thus the velocity field and the $\mathbf{B}$ matrix) can be obtained analytically and expressed as infinite series. Of course, the accuracy of calculated B_{ij}(t) depends on the number of terms in truncation of these infinite series. In the cases that the flow domain is not rectangular but the porous medium is still statistically homogeneous, a first-order analytical expression for matrix $\mathbf{B}$ may be derived using the potential theory (Lu and Zhang, 2003b). Though the potential is derived for homogeneous media with infinite extent and a mean uniform regional flow, the $\mathbf{B}$ matrix in this approach is independent of the mean uniform regional flow and depends only on the pumping (or injection) rate and the distance between the particle and well locations. When the particle is far away from the well, matrix $\mathbf{B}$ approaches zero, as is expected for the mean uniform regional flow. In this study, the above two approaches will be used to compute the $\mathbf{B}$ matrix and the resulted mean capture zones with confidence intervals will be compared with Monte Carlo results.

4 Construction of mean capture zones and confidence intervals

In our approach, the time-dependent well capture zones are determined by reverse particle tracking. For a flow field with pumping wells, streamlines (or pathlines for transient flow) converge to the wells and thus the flow field has singularities at the well locations. In the reverse particle tracking process, once a particle reaches a well, it is impossible to track it reversely and to tell where the particle came from. As a result, a small $r > 0$ is selected and the particles are released at a circle of radius r around each pumping well. Particles are arranged around each pumping well in such a way that more particles are on the down gradient direction of the mean uniform background flow. For example, if the uniform background flow is from the right to the left, more particles will be placed at the left side of the pumping wells. The mean trajectories $\langle \mathbf{X}_t \rangle$ and displacement covariances X_{ij} are then computed based on (7) and (8) for all particles released around all pumping wells. For a pumping well located at (x_{w1}, x_{w2}), the mean position $\langle \mathbf{X}_t \rangle$ and displacement covariance X_{ij} at any time for any released particle are then converted to the local polar coordinates centred at the well location. The first-order mean distance $\langle R \rangle$ from the well, its variance σ_R^2, and the first-order mean angle $\langle \theta \rangle$ from x_1 axis (pointed to the right) are computed from the mean trajectories and the displacement covariance according to the following formulae (Lu and Zhang, 2003b):

$$
\begin{aligned}
\langle R \rangle &= \sqrt{(\langle X_1 \rangle - x_{w1})^2 + (\langle X_2 \rangle - x_{w2})^2} \\
\sigma_R^2 &= \Big[(\langle X_1 \rangle - x_{w1})^2 X_{11} + 2(\langle X_1 \rangle - x_{w1})(\langle X_2 \rangle - x_{w2}) X_{12} \\
&\quad + (\langle X_2 \rangle - x_{w2})^2 X_{22} \Big] / \langle R \rangle^2 \\
\langle \theta \rangle &= \tan^{-1}\left(\frac{\langle X_2 \rangle - x_{w2}}{\langle X_1 \rangle - x_{w1}} \right)
\end{aligned}
\qquad (9)
$$

For any elapsed time, the convex hull that connects the endpoints of the mean trajectories ($\langle R \rangle$, $\langle \theta \rangle$) of all particles released around the well is considered the position of the mean capture zone for this well at the given time. The capture zone intervals at the 95% confidence level can be constructed by plus and minus $1.96\sigma_R$ on the mean capture zones, if the distribution of particles along radial directions at any given time is normal. If the distribution is not normal, the confidence intervals may be constructed using two quantiles $r_{0.025}$ and $r_{0.975}$. By quantile r_q, we mean that a q fraction of points is below the given value r_q. For example, the 0.975 quantile, $r_{0.975}$, is the value below which 97.5% of data fall and above which 2.5% of data fall. Lu and

Zhang (2003b) showed that the difference of confidence intervals derived from these two methods is not significant. As a result, in this paper, the capture zone intervals at the 95% confidence level are constructed using $\langle R \rangle$ plus and minus $1.96\sigma_R$ along the direction of the mean angle $\langle \theta \rangle$. As shown by Lu and Zhang (2003b), this approach is applicable to the situation of multiple wells.

5 Illustrative examples

To illustrate the proposed approach in determining well capture zones and examine the validity of the approach, we consider saturate flow in a rectangular domain of a heterogeneous porous medium. Although the developed model is applicable to solute transport in transient flow, for simplicity, we restrict our examples to steady-state flow conditions. The flow domain has a length $L_1 = 20$ (L) (where L is any consistent length unit) and a width $L_2 = 12$ (L), uniformly discretized into 50×30 square elements of a size 0.16 [L^2]. The statistics of the log hydraulic conductivity are given as $\langle Y \rangle = 0.0$(i.e., the geometric mean saturated hydraulic conductivity $K_G = 1.0$ [L T^{-1}], where T is any consistent time unit), $\sigma_Y^2 = 0.5$, $\lambda_Y = 2.0$ [L], which equals the length of five elements. The no-flow conditions are prescribed at two lateral boundaries. The hydraulic head is prescribed at the left and right boundaries as 10.0 [L] and 10.5 [L], respectively, which produces a background flow from the right to the left. A well with a pumping rate of $Q_w = 0.16$ [L^3 T^{-1}] is placed at (4.8 [L], 6.0 [L]).

For the purpose of comparison, we conduct Monte Carlo simulations. Using the random field generator, *sgsim*, developed by Deutsch and Journel (1998), we generate 5000 two-dimensional unconditional Gaussian realizations satisfying the above specifications. The saturated steady state flow equation is solved for each generated realization of the log hydraulic conductivity, using the Finite-Element Heat- and Mass-Transfer code (FEHM) developed by Zyvoloski et al. (1997). For each realization, once the flow field is solved, the velocity is negated and 42 non-reactive particles are placed on a circle of $r = 0.4$ [L] around the well. We then record each particle's position at some given times until it leaves the domain. Scatter plots of particles at some elapsed times in Monte Carlo simulations are compared against the mean capture zone and its confidence intervals at these times resulted from the ME approach.

In the illustrative example, we compare results of Monte Carlo simulations (scatter plots of particles at some given times) against the statistics of well capture zones (the mean and confidence intervals) computed from three different methods that distinguish from each other by the source of velocity statistics (from Monte Carlo simulations or the moment-equation approach) and by the way with which the transition matrix **B** is derived. In the first method, we use the sample mean velocity field and sample velocity covariances computed from Monte Carlo simulations as the input Eulerian mean velocity field and velocity covariances to the first-order stochastic transport model, i.e., Eqs. (7) and (8), but compute the transition matrix **B** using the potential theory. By using the velocity statistics from Monte Carlo simulations, we ensure that the stochastic transport model and the Monte Carlo transport simulations have the same underlying flow field and are thus compatible. The mean flow field is illustrated in Fig. 1, where the solid lines with arrows are streamlines. Particles are then released in the mean flow field at the same locations as in Monte Carlo simulations. The particles' mean (first-order) positions $\langle \mathbf{X}_t \rangle$ and their displacement covariances X_{ij} at any time then can be calculated using (7) and (8). The mean capture zones (white, solid curves) and confidence intervals (inner and outer curves, shown in dark and light, respectively) are constructed with the procedure described in the previous section and compared with Monte Carlo simulation results at two different times (Fig. 1). It is seen from the figures that mean capture zones and their associated uncertainties derived with this hybrid ME-MCS approach are in excellent agreement with the Monte Carlo results.

Figure 2 compares Monte Carlo simulation results (dots) and the mean capture zones with confidence intervals derived from using the flow statistics of Monte Carlo simulations while the **B** matrix computed using the first-order analytical solution (Lu and Zhang, 2003b), which is an infinite series. Though the results from the first-order transport model are in excellent agreement with Monte Carlo simulations, the agreement is not as good as in the previous case, because of the numerical errors (truncation errors) introduced in computing the **B** matrix. The accuracy of this method depends on the number of terms included in

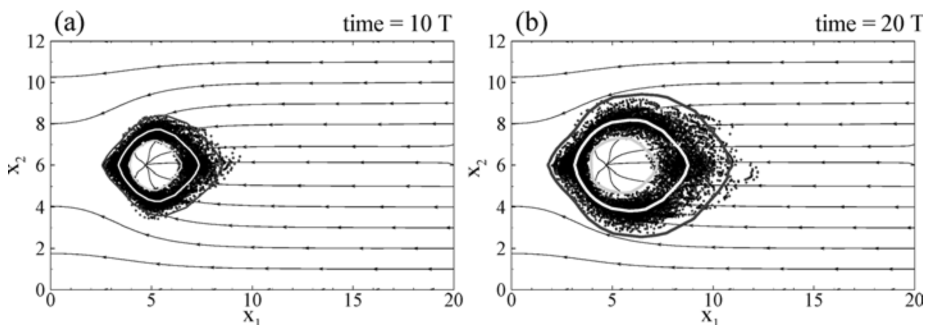


Fig. 1a,b Mean flow (streamlines) and comparisons of Monte Carlo simulations (dots) against the mean capture zones with confidence intervals derived using flow statistics from Monte Carlo simulations and the **B** matrix from the potential theory for two elapsed times. **a** $t = 10$ T and **b** t = 20 T, for $\sigma_Y^2 = 0.5$

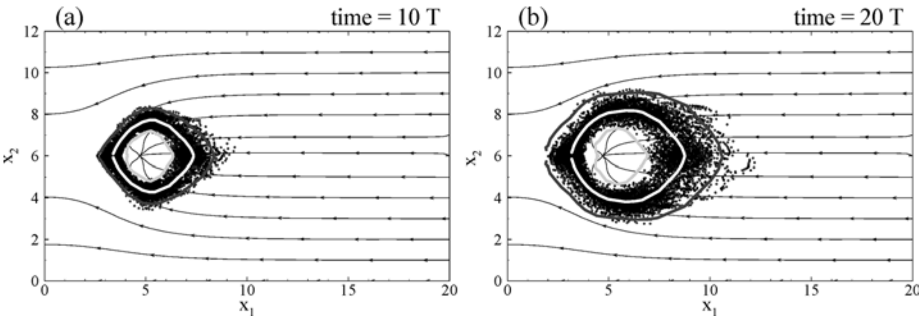


Fig. 2a,b Comparisons of Monte Carlo simulations (dots) against the mean capture zones with confidence intervals derived using flow statistics from Monte Carlo simulations and the **B** matrix from the analytical solution for two elapsed times. **a** $t = 10$ T and **b** $t = 20$ T, for $\sigma_Y^2 = 0.5$

approximating the **B** matrix. Besides, the computational demanding is high for this method than for the potential theory.

As the ME approach is an alternative to the computationally demanding Monte Carlo method, it is expected that the velocity statistics that are input to the moment transport model (7) and (8) should be derived directly from solving the flow moment equations, i.e., (4)–(6), rather than from Monte Carlo simulations. Figure 3 depicts comparisons of scatter plots of particle's positions from Monte Carlo simulations and the mean capture zones with confidence intervals derived using the flow statistics from the first-order ME approach while the **B** matrix is computed from the potential theory. Though in general the results from the first-order moment-equation approach are close to Monte Carlo results, the agreement between two approaches is not as good as in the previous two cases in which the velocity statistics from Monte Carlo simulations are used as input to first-order transport model. The major difference is on the mean capture zones, especially in the downstream direction. In this direction, the magnitude of the mean velocity computed from the moment-equation approach is slightly smaller than that from the Monte Carlo simulations. This may be due to errors induced in computing mean velocity in the first-order ME approach. In other words, the first-order ME approach is not accurate enough for this strongly non-uniform flow field with $\sigma_Y^2 = 0.5$ although literature results indicate that the first-order ME flow approach is robust for uniform mean flow, giving accurate results for σ_Y^2 as large as 4 (e.g., Zhang, 2002). If this is the case, it is expected that the agreement will be improved significantly for a smaller variability of log hydraulic conductivity. To verify this, we conduct the second numerical experiment by reducing the variability of log hydraulic conductivity from $\sigma_Y^2 = 0.5$ to $\sigma_Y^2 = 0.16$.

Figures 4 and 5 illustrate the comparisons of Monte Carlo simulation (MCS) results against the mean capture zones with confidence intervals derived using the velocity statistics from Monte Carlo simulations (Fig. 4) and from the first-order ME approach (Fig. 5). It is seen that at this variability of log hydraulic conductivity, the mean capture zones and the confidence intervals obtained by employing the velocity statistics from the ME approach are almost as good as those derived from

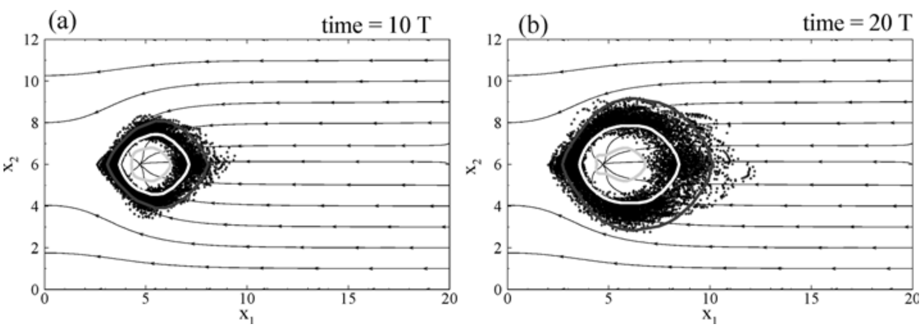


Fig. 3a,b Comparisons of Monte Carlo simulations (dots) against the mean capture zones with confidence intervals derived using flow statistics from the moment-equation approach and the **B** matrix from the potential theory for two elapsed times. **a** $t = 10$ T and **b** $t = 20$ T, for $\sigma_Y^2 = 0.5$

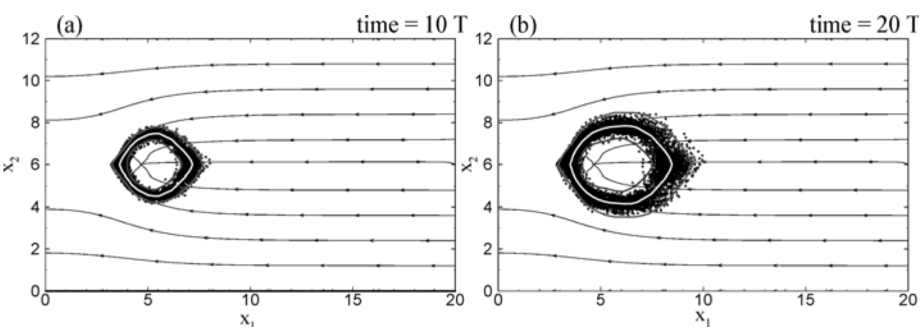
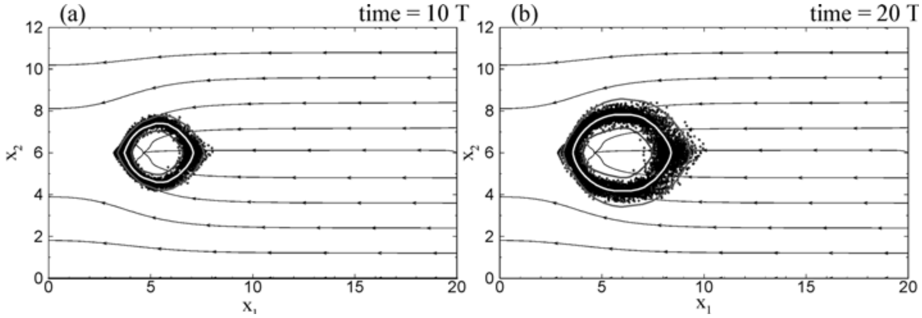


Fig. 4a,b Comparisons of Monte Carlo simulations (dots) against the mean capture zones with confidence intervals derived using flow statistics from Monte Carlo simulations and the **B** matrix from the potential theory for two elapsed times. **a** $t = 10$ T and **b** $t = 20$ T, for $\sigma_Y^2 = 0.16$

Fig. 5a,b Comparisons of Monte Carlo simulations (dots) against the mean capture zones with confidence intervals derived using flow statistics from the first-order moment-equation approach and the B matrix from the potential theory for two elapsed times. **a** t = 10 T and **b** t = 20 T, for $\sigma_Y^2 = 0.16$



using the velocity statistics of the Monte Carlo simulations.

There are two approximations in the full ME approach: One being associated with flow and the other being with transport. When the flow moments are given without approximation (using the Monte Carlo results), the ME based transport approach gives accurate results compared to the Monte Carlo transport approach at least for the variance of log hydraulic conductivity $\sigma_Y^2 = 0.5$ (Figs. 1 and 2). However, there exists a difference between the flow moments from the ME and MCS approaches for $\sigma_Y^2 = 0.5$ (not shown), which leads to the discrepancy in the delineation of the well capture zones (Fig. 3). A possible reason is that for porous media with a high variability on log hydraulic conductivity, the first-order ME approximations of flow statistics are not sufficiently accurate for strongly nonuniform flow fields as considered here. For such a flow field, higher-order corrections may be needed to render accurate flow moments even for the relatively small variability of $\sigma_Y^2 = 0.5$, contrary to uniform mean flows where the first-order ME approach is found to give reasonable results for σ_Y^2 as large as 4 (e.g., Zhang, 2002).

6 Summary and conclusions

It is possible to apply the stochastic moment-equation approach to construct time-dependent well capture zones and evaluate their uncertainties for multiple wells (pumping or injection) with a uniform mean background flow in bounded randomly heterogeneous porous media. The flow statistics can be obtained by solving the first two moments of flow, and the mean capture zones are determined using the mean velocity field by reversely tracking the non-reactive particles released at a small circle around each pumping well. The uncertainty associated with the mean capture zones is determined by the particle displacement covariance X_{ij} developed for nonstationary flow fields (Lu and Zhang, 2003a). We compared the scatter plots of particles' positions in Monte Carlo simulations against the mean capture zones with confidence intervals computed using flow statistics from both Monte Carlo simulations and the first-order moment equation (ME) approach. It is evident that, for a small variability of log hydraulic conductivity, the results from moment-equation approach are almost as good as those from Monte Carlo simulations, while the computational effort for the moment-equation approach is much less. When the variability of log hydraulic conductivity is relatively large, the results based on our moment approach deviate from the Monte Carlo results, especially in the downstream direction of pumping wells. A possible reason is that for porous media with a high variability of log hydraulic conductivity, the first-order ME approximations of flow statistics are not sufficiently accurate for strongly nonuniform flow fields as considered here. For such a flow field, higher-order corrections may be needed to render accurate flow moments even for relatively small variabilities of log hydraulic conductivity, contrary to uniform mean flows.

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